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## A coupled meshfree technique/molecular dynamics method for multiscale stress and deformation analysis in computational mechanics

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**Abstract:** A concurrent multiscale method has been developed based on the combination of the advanced meshfree method and molecular dynamics (MD). An advanced transition algorithm using regular transition particles was employed to ensure the compatibility of both displacements and their gradients. An effective local quasi-continuum approach is also applied to obtain the equivalent continuum strain energy density based on the atomistic potentials and Cauchy-Born rule. The influences of the size of transition region and the number of transition particles are investigated thoroughly. It has been demonstrated that the present multiscale simulation technique is very accurate and stable, and it has very good potential to develop a practical simulation tool for the multiscale systems in computational mechanics.

**Keywords:** Multiscale analysis; Meshfree method; Molecular dynamics; Coupling;

### 1 Introduction

Recently, one of the hottest topics in the computational mechanics is the multiscale modelling and simulation crossing macro/micro/nano dimensions, because, in many cases, it is essential to understand the properties of a deformation system across several length scales from macroscopic to microscopic to nanoscopic dimensions. It has produced many new challenges in the multiscale analyses. The existing numerical technique usually can only model the single scale, for example, the finite element method (FEM) for macro-scale, the molecular dynamics (MD) for atomic scale. There is no developed numerical tool, which can handle crossing scales at the same time. It is, therefore, necessary to develop an integrated multiscale modelling technique for the multiscale analysis. There have been significant efforts for the development of multiscale techniques since early 1970s. To date, a widely used multiscale technique is the coupling of FEM with MD analysis [1, 2]. However, because of the use of mesh in FEM, the application of FEM/MD has encountered many limitations.

Recently, various meshfree approaches [3, 4] have been proposed to overcome the disadvantages of FEM. Because the meshfree technique has many advantages, including: 1) no mesh required; 2) higher accuracy; 3) suitability for some difficult problems, etc., it seems have a good potential for multiscale analysis and have attracted the attention of the research community [5,6]. However, the research is still in its infancy and there are still many technical issues to resolve, including: a) more effective meshfree formulations for multiscale analyses; and b) reliable compatibility when bridging the dimensional scales. To overcome these problems, an advanced multiscale technique based on the meshfree/Molecular dynamics (MM) has been proposed by Gu and Zhang [7]. In their work, an advanced transition algorithm using regular transition particles was developed to ensure the compatibility of both displacements and their gradients, and, hence, it overcomes the shortcomings of the old handshaking algorithms. Through the use of the transition particles, the meshfree nodes and the MD atoms are totally independent resulting to reduce significantly the cost for node generation in the transition region. However, in this transition technique, there are some undefined parameters, e.g., the size of the transition region and the number of the transition particles. The selection of these parameters affects the performance of the multiscale technique, but the influence of them has not been thoroughly investigated.

In this paper, a concurrent multiscale method based on the combination of the advanced meshfree method and molecular dynamics (MD) is studied. The advanced transition algorithm using regular transition particles is employed to ensure the compatibility of both displacements and their gradients. In addition, an effective local quasi-continuum approach is also applied to obtain the equivalent continuum strain energy density based on the atomistic potentials and Cauchy-Born rule. The influences of the size of transition region and the number of transition particles are investigated thoroughly. The optimized ranges of these parameters are recommended. Numerical results have

demonstrated that the present multiscale simulation technique is very accurate and stable, and it has very good potential to develop a practical simulation tool for multiscale simulation in computational mechanics.

## 2 Transition technique

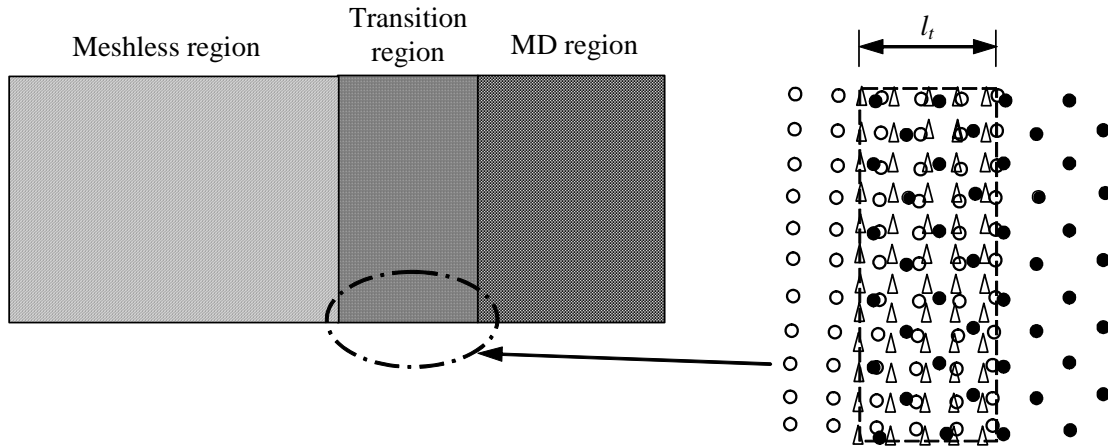
As shown in Figure 1, the problem domain is divided into the continuum domain  $\Omega_c$  and the atomic domain  $\Omega_a$ .  $\Omega_t$  is the transition domain between them. In  $\Omega_t$ , there are compatibility conditions for displacement and force equilibrium in coupling  $\Omega_c$  and  $\Omega_a$ :

$$\mathbf{u}_{k(c)} = \mathbf{u}_{k(a)}, \quad \mathbf{f}_{k(c)} + \mathbf{f}_{k(a)} = 0 \quad (1)$$

where  $\mathbf{u}_{k(a)}$ ,  $\mathbf{f}_{k(c)}$ ,  $\mathbf{u}_{k(a)}$ , and  $\mathbf{f}_{k(c)}$  are displacements and forces at a transition particle  $k$  obtained by the atomic method and continuum method, respectively.

To satisfy the displacement compatibility condition, several handshaking strategies have been developed [1, 2]. Following the idea of the bridging domain method [6], a newly developed transition technique [7] is developed to ensure a seamless transition between the continuum domain and the atomic domain. As shown in Figure 1, several layers of transition particles are inserted into  $\Omega_t$  to ensure the compatibility conditions and facilitate the energy exchange from  $\Omega_a$  to  $\Omega_c$ . The compatibility conditions between atoms and meshfree nodes are achieved through these transition particles. The kinetic energy and potential energy of continuum domain will first be transmitted to these transition particles and then to the atomic domain, and *vice versa*. This transition algorithm allows the continuum nodes to become independent of the atoms.

There are two important parameters, which are a)  $l_t$ , the size of the transition region; and b)  $N$ : the number of the transition particles, to affect the performance of this transition algorithm. Generally, to ensure the information transition between two domains, the transition region should be large enough. However, a larger transition region requires more transition particles and, hence, increases the computational cost. To find suitable values for these two parameters is one of key factors to improve the accuracy and efficiency of the multiscale simulation. These two parameters will be investigated in the following numerical studies.



**Figure 1** The computational multiscale modelling

## 3 The coupling method

The conservation of linear momentum for the continuum domain leads to

$$\nabla \cdot (\mathbf{S}\mathbf{F}^T) + \rho_0 \mathbf{b} = \rho_0 \ddot{\mathbf{u}}_{(c)} \quad (2)$$

where the subscript  $c$  denotes the variable for the continuum domain,  $\rho_0$  is the initial density,  $\mathbf{S}$  is the second Piola-Kirchhoff stress tensor which is often used in stress analysis because of symmetry,  $\mathbf{b}$  is the body force, and  $\ddot{\mathbf{u}}$  is the acceleration. Using the Lagrangian approach, we can get the Newton's equation of motion for the continuum domain,

$$m_{I(c)} \ddot{\mathbf{u}}_I = \mathbf{f}_{I(c)}^{\text{ext}} - \mathbf{f}_{I(c)}^{\text{int}} \quad (3)$$

where  $m_I^c$  is the lumped mass of the meshfree node  $I$ ,  $\mathbf{f}_{I(c)}^{\text{ext}}$  is the external force subjected to node  $I$ , and the internal force,  $\mathbf{f}_{I(c)}^{\text{int}}$ , can be obtained by

$$\mathbf{f}_{I(c)}^{\text{int}} = \int_{\Omega_0^c} \frac{\partial w_{(c)}}{\partial \mathbf{u}_{I(c)}} d\Omega = \int_{\Omega_0^c} \frac{\partial w_{(c)}}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\partial \mathbf{u}_{I(c)}} d\Omega = \int_{\Omega_0^c} \frac{\partial \Phi_I}{\partial \mathbf{X}} \mathbf{F} \mathbf{S}_{(c)} d\Omega \quad (4)$$

where  $\Phi$  is the meshfree shape functions which are constructed using the radial basis interpolation [4].

Implying the conservation of energy and the MD trajectories, the Newton's equation of motion for the MD analysis can be obtained

$$m_{i(a)} \ddot{\mathbf{u}}_{i(a)} = \mathbf{f}_i^a = \mathbf{f}_{i(a)}^{\text{ext}} - \mathbf{f}_{i(a)}^{\text{int}} \quad (5)$$

where  $m_i$  is the mass of the atom  $i$ ,  $\ddot{\mathbf{u}}_{i(a)}$  is the acceleration of atom  $i$ ,  $\mathbf{f}_{i(a)}^{\text{ext}}$  is the external force subjected to atom  $i$ , and  $\mathbf{f}_{i(a)}^{\text{int}}$  is the internal force with  $\mathbf{f}_{i(a)}^{\text{int}} = \partial w_{(a)} / \partial \mathbf{u}_{i(a)}$ .

The constitutive equation for the continuum domain can be constructed using the Cauchy–Born rule locally, and therefore, the second Piola-Kirchhoff stress can be obtained from

$$\mathbf{S} = \frac{\partial \mathbf{w}_{(c)}}{\partial \mathbf{C}} = \frac{\partial \mathbf{w}_{(c)}}{\partial (\mathbf{F}^T \mathbf{F})}, \text{ where } w_{(c)} = \frac{1}{V_{v(c)}} \left[ \sum w_{jv(a)}(\mathbf{r}) - \sum w_{jv(a)}(\mathbf{r}_0) \right] \quad (6)$$

where  $w_{(c)}$  is the potential energy per unit volume of the continuum, which depends on the elongations and angle changes of the atomic bonds,  $V_{v(c)}$  is the volume of the virtual representative-cell,  $w_{jv(a)}(\mathbf{r})$  is the potential energy of atom  $j$  after deformation, and  $w_{jv(a)}(\mathbf{r}_0)$  is the potential energy of atom  $j$  in the unstrained (undeformed) state. To improve the computational efficiency and robustness, we use the virtual representative-cell method [7] in this paper.

The generalized displacement and its derivative of a transition particle at  $\mathbf{x}_I$  can be defined as

$$\begin{cases} \mathbf{g}_I = \mathbf{u}^c(\mathbf{x}_I) - \mathbf{u}^a(\mathbf{x}_I) = \sum_I \Phi_I(\mathbf{x}_I) \mathbf{u}_I^c - \sum_i \Phi_i(\mathbf{x}_I) \mathbf{u}_i^a \\ \mathbf{g}_{I(x)} = \frac{\partial \mathbf{u}^c(\mathbf{x}_I)}{\partial \mathbf{x}^c} - \frac{\partial \mathbf{u}^a(\mathbf{x}_I)}{\partial \mathbf{x}^a} = \sum_I \frac{\partial \Phi_I(\mathbf{x}_I)}{\partial \mathbf{x}^c} \mathbf{u}_I^c - \sum_i \frac{\partial \Phi_i(\mathbf{x}_I)}{\partial \mathbf{x}^a} \mathbf{u}_i^a \end{cases} \quad (7)$$

where  $\mathbf{u}^c(\mathbf{x}_I)$  and  $\mathbf{u}^a(\mathbf{x}_I)$  are the displacements of the transition particle at  $\mathbf{x}_I$  obtained by the interpolations using continuum nodes and atoms, respectively, and  $\Phi$  is the meshfree shape function.

To ensure the conservation of mass and energy, using the method developed by Xiao and Belytschko [6], the total energy and mass are taken to be linear distributions using a scaling parameter  $\alpha$  in the transition domain. The Hamiltonian for the total problem domain is the linear combination of the atomic, continuum and the constrain terms of transition particles, i.e.,

$$H = (1 - \alpha) H^a + \alpha H^c + H^m = (1 - \alpha) H^a + \alpha H^c + \sum_I \beta_I^{(1)} \mathbf{g}_I + \sum_I \beta_I^{(2)} \mathbf{g}_I^T \mathbf{g}_I + \sum_I \beta_I^{(3)} \mathbf{g}_{I(x)}^T \mathbf{g}_{I(x)} \quad (8)$$

where  $\beta_I^{(1)}$ ,  $\beta_I^{(2)}$ , and  $\beta_I^{(3)}$  are penalty coefficients for the transition point  $I$ .

Hence, the equations (3) and (5) of motions for continuum and atomic domains can be re-written as

$$\begin{aligned} m_{I(c)} \ddot{\mathbf{u}}_{I(c)} &= \mathbf{f}_{I(c)} = \mathbf{f}_{I(c)}^{\text{ext}} - \left( \mathbf{f}_{I(c)}^{\text{int}} + \frac{\mathbf{f}_{I(c)}^{\text{tran}} + \mathbf{f}_{I(c)}^{\text{tran}(x)}}{\alpha(\mathbf{X}_I)} \right), \\ m_{i(a)} \ddot{\mathbf{u}}_{i(a)} &= \mathbf{f}_{i(a)} = \mathbf{f}_{i(a)}^{\text{ext}} - \left( \mathbf{f}_{i(a)}^{\text{int}} + \frac{\mathbf{f}_{i(a)}^{\text{tran}} + \mathbf{f}_{i(a)}^{\text{tran}(x)}}{1 - \alpha(\mathbf{X}_i)} \right) \end{aligned} \quad (9)$$

where  $\mathbf{f}_{I(c)}^{\text{tran}}$ ,  $\mathbf{f}_{I(c)}^{\text{tran}(x)}$ ,  $\mathbf{f}_{i(a)}^{\text{tran}}$  and  $\mathbf{f}_{i(a)}^{\text{tran}(x)}$  are constraint forces due to the penalty terms to enforce the displacement and its derivative compatibility conditions for the continuum and atomic domain, respectively, i.e.

$$\mathbf{f}_{I(c)}^{\text{tran}} = \sum_l \beta_l^{(1)} \Phi_{II} \mathbf{I} + \sum_l \beta_l^{(2)} \left[ \sum_l \Phi_l(\mathbf{x}_l) \mathbf{u}_l^c - \sum_i \Phi_i(\mathbf{x}_l) \mathbf{u}_i^a \right] [\Phi_{II} \mathbf{I}]; \quad \mathbf{f}_{I(c)}^{\text{tran}(x)} = \sum_l \beta_l^{(3)} \Phi_{II,x} \mathbf{I} \quad (10)$$

$$\mathbf{f}_{i(a)}^{\text{tran}} = -\sum_l \beta_l^{(1)} \Phi_{il} \mathbf{I} - \sum_l \beta_l^{(2)} \left[ \sum_l \Phi_l(\mathbf{x}_l) \mathbf{u}_l^c - \sum_i \Phi_i(\mathbf{x}_l) \mathbf{u}_i^a \right] [\Phi_{il} \mathbf{I}]; \quad \mathbf{f}_{i(a)}^{\text{tran}(x)} = -\sum_l \beta_l^{(3)} \Phi_{il,x} \mathbf{I} \quad (11)$$

Since the frequency of the atomic domain is much higher than that of the continuum domain, the multiple-time-step algorithm is more favorable, both computationally and physically. Hence, we will use this algorithm, in which a larger time step is used in the continuum domain but a finer time step is used in the atomic domain. Let  $\Delta T^c$  be the time step for the continuum domain and  $\Delta t^a$  be the time step for the atomic domain. We use  $\Delta T^c = M \Delta t^a$ . Therefore, the velocity Verlet integrator can be rewritten as,

$$\mathbf{u}_{I(n+1)} = \mathbf{u}_{I(n)} + \dot{\mathbf{u}}_{I(n)} \Delta T + \frac{1}{2} \frac{\mathbf{f}_{I(n)}}{m_I} \Delta T^2, \quad \dot{\mathbf{u}}_{I(n+\frac{j+1}{M})} = \dot{\mathbf{u}}_{I(n+\frac{j}{M})} + \frac{\Delta t}{2m_I} \left( \mathbf{f}_{I(n+\frac{j}{M})} + \mathbf{f}_{I(n+\frac{j+1}{M})} \right), \quad \text{in } \Omega_{(c)} \quad (12)$$

$$\mathbf{u}_{i(n+\frac{j+1}{M})} = \mathbf{u}_{i(n+\frac{j}{M})} + \dot{\mathbf{u}}_{i(n+\frac{j}{M})} \Delta t + \frac{1}{2} \frac{\mathbf{f}_{i(n+\frac{j}{M})}}{m_i} \Delta t^2, \quad \dot{\mathbf{u}}_{i(n+\frac{j+1}{M})} = \dot{\mathbf{u}}_{i(n+\frac{j}{M})} + \frac{\Delta t}{2m_i} \left( \mathbf{f}_{i(n+\frac{j}{M})} + \mathbf{f}_{i(n+\frac{j+1}{M})} \right), \quad \text{in } \Omega_{(a)} \quad (13)$$

where  $j = 0 \sim M-1$ . The above equations indicate that the variables in the atomic domain will be repeatedly calculated for  $M$  times at the finer time step to match the coarse time step in the continuum domain.

## 4 Numerical Results and Discussions

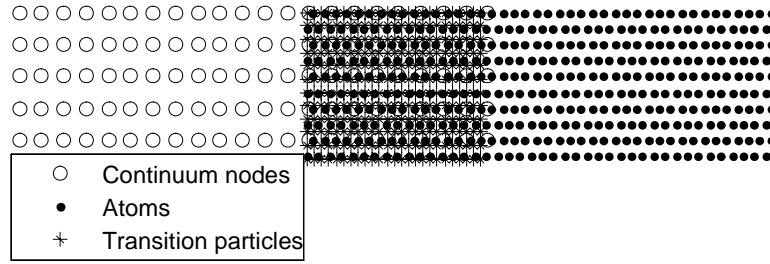
Here we examine the wave propagation in a two-dimensional grapheme sheet whose thickness is a single atom layer, and Lennard-Jones (L-J) 6-12 Interatomic potential [7] is used. For comparison, the problem is also simulated by pure MD and the relative error between the MD and our multiscale results is measured by the following error indicator

$$e = \left| \sum_i^m |u_i^{\text{MD}}| - \sum_i^m |u_i^{\text{MM}}| \right| / \left| \sum_i^m |u_i^{\text{MD}}| \right| \quad (14)$$

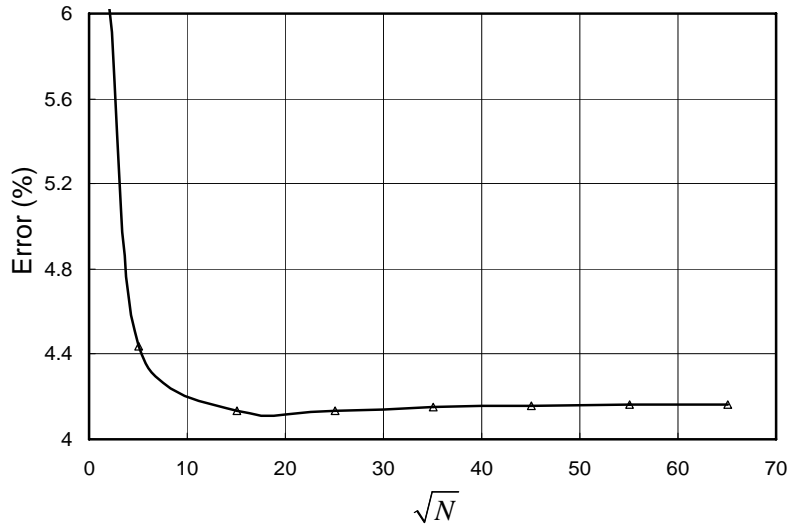
where  $u_i^{\text{MD}}$  and  $u_i^{\text{MM}}$  are displacement at the  $i$ th atom in the atomic domain obtained using the MD and our MM method, respectively;  $m$  is the number of atoms in the atomic sub-domain.

The initial displacement is taken as a quarter of sinusoid, and applied on the right portion of the atomic domain. The periodic boundary condition is applied along the vertical direction. The coupling model of this 2-D sheet is shown in Figure 2. The length of the transition region is 1.95 nm, which is represented by regularly distributed transition particles. The time step for the atomic domain is  $\Delta t_{(a)} = 0.005$ ps, and the multiple time step factor  $M$  is 5.

The average errors for different numbers of transition particles are illustrated in Figure 3, where we can see that the computational results are stable when the number is large enough ( $>25$  for this problem). Too few transition particles cannot ensure the compatibility accuracy, and hence lead to a large computational error. On the other hand, if the transition particles are too many, it will significantly increase the computational time without noticeable accuracy improvement. Hence, the number of transition particles should be considered to maximise the computation efficiency with acceptable accuracy. For the present example,  $N=225\sim600$  are a good selection.



**Figure 2** Multiscale computational model



**Figure 3** Influences of the number of transition particles  $N$

To investigate the influence of the size of the transition region, we define  $l_t = \alpha \cdot d_{(a)}$ , where  $d_{(a)}$  is the space between two atoms. Figure 4 plots the computational errors vs. the dimensionless parameter  $\alpha$ . From this figure, we can find that the transition region should be large enough to ensure the compatibility. However, a larger transition region requires more transition particles and, hence, increases the computational cost. For this study,  $\alpha = 5 \sim 20$  is a reasonable choice.

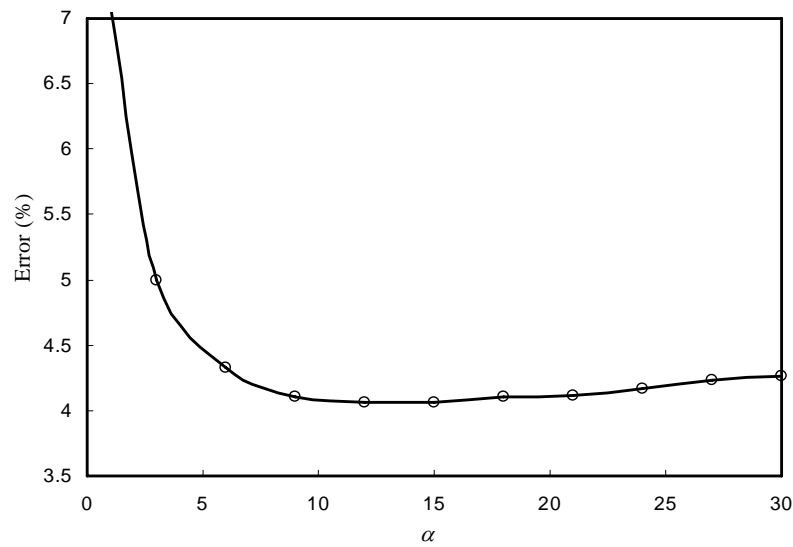
Using the parameters obtained from above studies, Figure 5 shows the energy transfer between the continuum and atomic sub-domains. It demonstrates that all the energy in atomic sub-domain has been transferred into the continuum sub-domain through our transition technique.

## 5 Conclusion

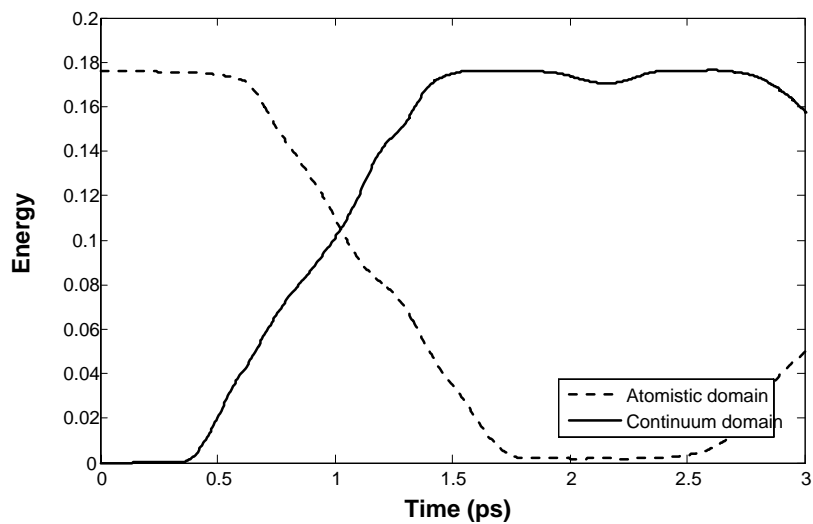
A novel concurrent multiscale method, which is based on the combination of the advanced meshfree method and molecular dynamics (MD), is studied. An advanced transition algorithm using regular transition particles was employed to ensure the compatibility of both displacements and their gradients. In addition, an effective local quasi-continuum approach is also applied to obtain the equivalent continuum strain energy density based on the atomistic potentials and Cauchy-Born rule. The influences of the size of transition region and the number of transition particles are investigated thoroughly. The number of transition particles,  $N$ , is recommended  $N=225\sim600$ , and the dimensionless parameter  $\alpha$  for the size of transition region is recommended  $\alpha = 5 \sim 20$ . Numerical studies have demonstrated that the present multiscale simulation technique is very accurate and stable, and it has very good potential to develop a practical simulation tool for the multiscale simulations in engineering.

## Acknowledgement:

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**Figure 4** Influences of dimensionless parameter  $\alpha$  for the size of transition region



**Figure 5** Energy transfer between the continuum and atomic domains

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